

Probability distributions for Markov chains based quantum walks

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Abstract

We analyze the probability distributions of the quantum walks induced from Markov chains by Szegedy (2004). The first part of this paper is devoted to the quantum walks induced from finite state Markov chains. It is shown that the probability distribution on the states of the underlying Markov chain is always convergent in the Cesaro sense. In particular, we deduce that the limiting distribution is uniform if the transition matrix is symmetric. In the cases of non-symmetric Markov chain, we exemplify that the limiting distribution of the quantum walk is not necessarily identical with the stationary distribution of the underlying irreducible Markov chain. The Szegedy scheme can be extended to infinite state Markov chains (random walks). In the second part, we formulate the quantum walk induced from a lazy random walk on the line. We then obtain the weak limit of the quantum walk. It is noted that the quantum walk appears to spread faster than its counterpart-quantum walk on the line driven by the Grover coin discussed in literature. The paper closes with an outlook on possible future directions.

1 Introduction

Random walks have proved to be a fundamental mathematical tool for modeling and simulating complex problems and natural phenomena. Among the various applications of random walks we find the development of stochastic algorithms [1, 2] for problems of paramount importance in theoretical computer science [3], earthquake modeling [4], computer vision [5], financial modeling [6], graph theory [7], proteomics [8, 9] and Internet technology [10, 11, 12, 13].

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As a quantum mechanical counterpart of random walks, in recent times quantum walks [14, 15, 16, 17, 18, 19, 20] have been extensively studied. Quantum walks were originally devised under the same rationale as classical random walks, as a mathematical basis to develop sophisticated algorithms (e.g. [21, 22, 23, 24, 25, 26]). Unlike the random walks formulated by iteration of probability transition matrices on a probability distribution, quantum walks are defined by unitary evolutions of the *probability amplitudes*. The resulting probability distribution is defined to be the sum of squares of the norms of amplitudes so that there exists a non-linearity map between the initial state and the resulting probability distribution. Due to their inherent nonlinear chaotic dynamic behavior and quantum interference effects, quantum walks have been shown to outperform random walks at certain computational tasks [21, 22, 24, 27, 28, 29, 30, 31, 32, 33]; moreover, it has been proved that both continuous and discrete quantum walks constitute universal models of quantum computation [34, 35]. For a lively and informative elaboration of the history of quantum walks and their connection to quantum computing, physics and the natural sciences, the reader is referred to [36, 37, 38, 39, 40, 41, 42] and the references therein.

We distinguish between two types of QW: *continuous time* and *discrete time*. In both cases, quantum walks are run on graphs (i.e., on discrete spaces) but their evolution timing is different: as for continuous quantum walks, evolution is described by the Schrödinger equation whose Hamiltonian is built based on the Laplacian matrix of the graph where the quantum walk is run on [16]; as for discrete quantum walks, evolution is described by unitary operators that are applied in discrete time steps [17, 18, 20].

As for discrete-time quantum walks, in addition to the “position” register, an extra register is needed to store the direction in which the walker unitarily moves from a node to its neighboring nodes. Two important types of discrete-time quantum walks have been studied:

- **Coin-driven quantum walks (coin-driven QW).** This model of quantum walk, initially proposed by [17, 18], is composed of two quantum systems: i) a walker, which is a quantum system living in a Hilbert space of finite or infinite but countable dimension \mathcal{H}_p , and ii) a coin, which is a quantum system living in a 2-dimensional Hilbert space \mathcal{H}_c . The unitary maps in the framework of coin-driven QW are defined in terms of conditional shifts and coin operators, by which the evolution of the pure state of the quantum system is governed.
- **Markov chain-based quantum walks (MCBQW).** The other type of discrete-time quantum walk was proposed by [20] where both registers are nodes. The corresponding unitary map in this scenario is given by a swap operator and a *reflection operator* in

the Hilbert space. It is noted that the reflection operator is derived by *quantizing* a Markov chain associated with the underlying graph.

Although MCBQW have been studied in some detail by the scientific community (see, for example, [43, 44, 45, 46] and the references therein), many mathematical, statistical and computational properties of MCBQW remain to be discovered, like the asymptotic average probability distributions of MCBQW on a general finite graph that, so far, remain largely unexplored. Moreover, results on probability distributions and properties of the underlying Markov chains have been barely explored. For instance:

- It is unknown whether MCBQW constitute a model of universal quantum computation or if it is equivalent to a more modest model of quantum computation like quantum annealing [47].
- In [48], the authors propose a class of quantum PageRank algorithms and introduce an instance of this class. Since the original formulation of PageRank can be described in terms of Markov chains [10, 11, 12, 13], the class of quantum PageRank algorithms introduced in [48] is required to admit a quantized Markov chain description. With the purpose of mathematically characterizing the behavior of this quantum PageRank instance, two notions are proposed: the instantaneous importance $I_q(P_i, m)$ of a quantum web page P_i (that is, the quantum PageRank of P_i) be equal to the probability of finding the quantum walker at node i after m time steps. Due to unitary evolution, $I_q(P_i, m)$ does not converge, hence the notion of average probability $\bar{P}_T(j|\alpha_0)$ is introduced. Interesting numerical results related to the properties of quantum PageRank on some graphs are presented; however, no asymptotic analytical results are shown.
- In [49], although the asymptotic average probability distributions were derived, their discussion is only confined to the MCBQW on a finite *path*.
- In [50], the author managed to treat the relationship between the localization of MCBQW and the recurrent properties of the underlying Markov chains on a *half line*. To the best of our knowledge, this is the only publication in which the inherent connection between the statistical properties of MCBQW and the properties of underlying Markov chains are examined.

As an effort to address important fronts related to MCBQW, in this paper we analyze the asymptotic probability distributions of MCBQW. In particular, we deduce that the

limiting distribution is uniform if the transition matrix is symmetric. In the cases of non-symmetric Markov chain, we exemplify that the limiting distribution of the quantum walk is not necessarily identical with the stationary distribution of the underlying irreducible Markov chain. The Szegedy scheme [20] can be extended to infinite state Markov chains. In the second part, we formulate the quantum walk induced from a lazy random walk on the line. We then obtain the weak limit of the quantum walk. It is noted that the quantum walk appears to spread faster than its counterpart-quantum walk on the line driven by the Grover coin discussed in literature. The paper closes with an outlook on possible future directions.

2 Preliminaries

Szegedy developed a general method for quantizing a Markov chain to create a discrete-time quantum walk [20]. Let $P = (p_{jk})$ be an $n \times n$ stochastic matrix representing the transition probability matrix of a Markov chain on a directed graph $G(V, E)$. Here V is the set of the vertices of G , E is the set of the oriented edge of G , $E = \{(j, k) : j, k \in V\}$. In order to introduce a discrete-time quantum walk on the same graph we use as the Hilbert space of the QW the span of all vectors representing the $n \times n$ (directed) edges of the graphs, i.e., $\mathcal{H} = \text{span}\{|j\rangle \otimes |k\rangle, j, k \in V\}$.

Let us define the vector states: $|\psi_j\rangle = \sum_{k=1}^n \sqrt{p_{jk}} |j\rangle \otimes |k\rangle$, which is a superposition of the vectors representing the edges outgoing from the j^{th} vertex. The weights are given by (the square root of the entries of) the transition matrix P .

One can easily verify that due to the stochasticity of P , $\{|\psi_j\rangle\}_{j=1}^n$ is an orthonormal set in \mathcal{H} . The operator $\Pi = \sum_{j=1}^n |\psi_j\rangle\langle\psi_j|$, is then an orthogonal projector onto the subspace $\mathcal{H}_\psi = \text{span}\{|\psi_j\rangle : j \in V\}$. With this, a single step of the quantum walk is then given by the unitary operator $U := S(2\Pi - 1)$ where $S = \sum_{j,k} |j \otimes k\rangle\langle k \otimes j|$ is the swap operator.

Given $|\alpha_0\rangle \in \mathcal{H}$, where $\| |\alpha_0\rangle \| = 1$, the expression $|\alpha_t\rangle = U^t |\alpha_0\rangle$ is called the state for the walk at time t . The corresponding quantum walk (MCBQW) with the initial state $|\alpha_0\rangle$ is represented by the sequence $\{|\alpha_t\rangle\}_{t=0}^\infty$.

Indeed, the structure of operator $U := S(2\Pi - 1)$ resembles Grover's diffusion operator [51]. Analysis on this regard have been presented in [52, 53]. Also, a step-by-step introduction to Szegedy's quantum walks together with a detailed example of this kind of quantum walks on a 3×3 lattice is presented in [54].

In order to analyze the MCBQW, we need to study the spectral properties of an $n \times n$ matrix $D = (d_{jk})$, which can be viewed as a linear transformation on the space $\mathcal{H}_V = \mathbb{C}^n = \text{span}\{|j\rangle : j \in V\}$ and indeed builds a bridge from the classical Markov chain to the quantum walk. This matrix is defined as follows:

$$d_{jk} = \sqrt{p_{jk}p_{kj}}. \quad (1)$$

Let us then define an operator A from the space \mathcal{H}_V to \mathcal{H}_ψ :

$$A = \sum_{j=1}^n |\psi_j\rangle\langle j|$$

The following identities describe the relationships among these operators:

$$A^\dagger A = \mathbb{I}, AA^\dagger = \Pi, A^\dagger SA = D$$

Since D is symmetric by its definition, without loss of the generality, we may assume that, via the Spectral Decomposition, $D = \sum_r \lambda_r |w_r\rangle\langle w_r| + \sum_s |u_s\rangle\langle u_s| - \sum_t |v_t\rangle\langle v_t|$ where $\lambda_r (\neq \pm 1)$, 1 and -1 are the eigenvalues of D , $\{|w_r\rangle, |u_s\rangle, |v_t\rangle\}$ is an *orthonormal* basis for \mathcal{H}_V . Each $|w_r\rangle$ is an eigenvector of D with eigenvalue λ_r , $|u_s\rangle$ and $|v_t\rangle$ are eigenvectors of D with eigenvalues 1 and -1 , respectively. It should be pointed out that each $\lambda_r \in (-1, 1)$ by the construction of the matrix D . Since $A^\dagger A = \mathbb{I}$, $\{A|w_r\rangle, A|u_s\rangle, A|v_t\rangle\}$ is an orthonormal basis for \mathcal{H}_ψ . Thus, the subspace $\mathcal{H}_{\psi,S} = \text{span}\{|\psi_j\rangle, S|\psi_j\rangle : j \in V\}$ is identical with the subspace $\text{span}\{A|w_r\rangle, SA|w_r\rangle, A|u_s\rangle, SA|u_s\rangle, A|v_t\rangle, SA|v_t\rangle\}$, which is invariant under the unitary operator U . The spectral structure of unitary operator U is intimately connected with the matrix D :

1. $A|w\rangle - e^{\pm i \arccos \lambda_r} SA|w\rangle$ are eigenvectors of U with eigenvalues $e^{\pm i \arccos \lambda_r}$, respectively.
2. $A|u\rangle = SA|u\rangle$, and $A|u\rangle$ is an eigenvector of U with eigenvalue 1.
3. $A|v\rangle = -SA|v\rangle$, and $A|v\rangle$ is an eigenvector of U with eigenvalue -1 .

Items 2 and 3 imply that the invariant subspace of U , $\mathcal{H}_{\psi,S} = \text{span}\{A|w_r\rangle, SA|w_r\rangle, A|u_s\rangle, A|v_t\rangle\}$.

It is straightforward to verify that $\{A|w_r\rangle - e^{\pm i \arccos \lambda_r} SA|w_r\rangle, A|u_s\rangle, A|v_t\rangle\}$, the collection of all these eigenvectors of U , forms an orthogonal set. Moreover, $\|A|u\rangle\| = \|A|v\rangle\| = 1$ and $\|A|w_r\rangle - e^{\pm i \arccos \lambda_r} SA|w_r\rangle\| = \sqrt{2 - 2\lambda_r^2}$.

Since the set of vectors $A|w_r\rangle, SA|w_r\rangle, A|u_s\rangle, A|v_t\rangle$ are linearly independent, $\mathcal{H}_{\psi,S}$ is in fact identical with the subspace

$$\text{span}\{A|w_r\rangle - e^{\pm i \arccos \lambda_r} SA|w_r\rangle, A|u_s\rangle, A|v_t\rangle\},$$

$$\text{i.e., } \mathcal{H}_{\psi,S} = \text{span}\{A|w_r\rangle - e^{\pm i \arccos \lambda_r} SA|w_r\rangle, A|u_s\rangle, A|v_t\rangle\}.$$

We set

1. $A|w_r^+\rangle = (A|w_r\rangle - e^{i \arccos \lambda_r} SA|w_r\rangle)/\sqrt{2 - 2\lambda_r^2}$
2. $A|w_r^-\rangle = (A|w_r\rangle - e^{-i \arccos \lambda_r} SA|w_r\rangle)/\sqrt{2 - 2\lambda_r^2}$

Then the invariant subspace of U is identical to the subspace $\text{span}\{A|w_r^+\rangle, A|w_r^-\rangle, A|u_s\rangle, A|v_t\rangle\}$. This is a subspace spanned by the set of orthonormal eigenvectors of U associated with the key operator D .

Let us decompose the Hilbert space \mathcal{H} into $\mathcal{H}_{\psi,S}$ and its orthogonal complement $\mathcal{H}_{\psi,S}^\perp$, i.e., $\mathcal{H} = \mathcal{H}_{\psi,S} \oplus \mathcal{H}_{\psi,S}^\perp$. It is not difficult to check that the action of U on $\mathcal{H}_{\psi,S}^\perp$ is exactly $-S$ and this subspace is invariant under U , thereby U^2 just trivially acts on the subspace as an identity. The nontrivial dynamics of U only takes place on the subspace $\mathcal{H}_{\psi,S}$. By its construction, the dimension of the subspace $\mathcal{H}_{\psi,S}$ is at most $2n$ (the dimension of the whole space \mathcal{H} is n^2), which can be achieved only if D does not have both 1 and -1 as its eigenvalues. Based on the aforesaid observation, we may confine the initial state of the quantum walk to the subspace $\mathcal{H}_{\psi,S}$, which is spanned by the set of the orthonormal eigenvectors of U : $\{A|w_r^+\rangle, A|w_r^-\rangle, A|u_s\rangle, A|v_t\rangle\}$.

For the sake of better exposure of our main result, we relabel the above orthonormal eigenvectors of U , which forms a basis for the invariant subspace $\mathcal{H}_{\psi,S}$, as $\{|\phi_l\rangle\}$ with associated eigenvalues $\{\mu_l\}$, $l = 1, 2, \dots, m$ where $m \leq 2n$.

3 Asymptotic distribution on the states of the underlying Markov chain

We now proceed to study the evolution of the quantum walk as a function of time. Provided that the initial state $|\alpha_0\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |\psi_j\rangle$, then the state of the quantum walk at time t is $|\alpha_t\rangle = U^t |\alpha_0\rangle$. Since U is unitary, in general $\lim_{t \rightarrow \infty} |\alpha_t\rangle$ does not exist. Now consider instead the probability distribution on the states of the underlying Markov chain induced by $|\alpha_t\rangle$,

Definition. $P_t(j|\alpha_0) = \sum_k |\langle j \otimes k | \alpha_t \rangle|^2$.

As a matter of fact, P_t does not converge either. However, the average of P_t over time would converge. We define:

Definition. $\bar{P}_T(j|\alpha_0) = \frac{1}{T} \sum_{t=1}^T P_t(j|\alpha_0)$.

We shall give an explicit formula for the limit of \bar{P}_T .

Theorem 1 Given a Markov chain on the state space V with the transition matrix P , the induced quantum walk is defined as $|\alpha_t\rangle = U^t |\alpha_0\rangle$ where the initial state $|\alpha_0\rangle = \sum_l \langle \phi_l | \alpha_0 \rangle |\phi_l\rangle$, then

$$\bar{P}_\infty(j|\alpha_0) = \lim_{T \rightarrow \infty} \bar{P}_T(j|\alpha_0) = \sum_k \sum_{l,m} \langle \phi_l | \alpha_0 \rangle \langle j \otimes k | \phi_l \rangle \langle \alpha_0 | \phi_m \rangle \langle \phi_m | j \otimes k \rangle$$

where the first sum is over all values of k , and the second sum is only on pairs l, m such that $\mu_l = \mu_m$.

Proof Note that $|\alpha_t\rangle = U^t |\alpha_0\rangle = \sum_l \langle \phi_l | \alpha_0 \rangle \mu_l^t |\phi_l\rangle$, then one has

$$|\alpha_t\rangle \langle \alpha_t| = \sum_l \sum_m \langle \phi_l | \alpha_0 \rangle \overline{\langle \phi_m | \alpha_0 \rangle} (\mu_l \bar{\mu}_m)^t |\phi_l\rangle \langle \phi_m|.$$

Since $\bar{P}_T(j|\alpha_0) = \frac{1}{T} \sum_{t=1}^T P_t(j|\alpha_0) = \frac{1}{T} \sum_{t=1}^T \sum_k |\langle j \otimes k | \alpha_t \rangle|^2$,

$$\bar{P}_T(j|\alpha_0) = \frac{1}{T} \sum_{t=1}^T \sum_k \sum_l \sum_m \langle \phi_l | \alpha_0 \rangle \overline{\langle \phi_m | \alpha_0 \rangle} (\mu_l \bar{\mu}_m)^t \langle j, k | \phi_l \rangle \langle \phi_m | j, k \rangle \quad (2)$$

We separate the sum in the right-hand side of Eq.(2) into two parts: One part in which $\mu_l = \mu_m$, this part is $\sum_k \sum_l \sum_m \langle \phi_l | \alpha_0 \rangle \overline{\langle \phi_m | \alpha_0 \rangle} \langle j, k | \phi_l \rangle \langle \phi_m | j, k \rangle$. The other part in which $\mu_l \neq \mu_m$ can be written as $\sum_k \sum_l \sum_m \frac{\mu_l \bar{\mu}_m [1 - (\mu_l \bar{\mu}_m)^T]}{T(1 - \mu_l \bar{\mu}_m)} \langle \phi_l | \alpha_0 \rangle \overline{\langle \phi_m | \alpha_0 \rangle} \langle j, k | \phi_l \rangle \langle \phi_m | j, k \rangle$.

It can be seen that the latter part converges to zero as T goes to infinity. The only contribution to the limit of the average probability $\bar{P}_T(j|\alpha_0)$ comes from the part with $\mu_l = \mu_m$. This completes the proof.

When the transition matrix P of a Markov chain is symmetric, the limiting probability is uniform. This assertion is recorded in the theorem below.

Theorem 2 Given a Markov chain on the state space V with a symmetric transition matrix P , the induced quantum walk is defined as $|\alpha_t\rangle = U^t|\alpha_0\rangle$ where the initial state $|\alpha_0\rangle = \sum_l \langle \phi_l | \alpha_0 \rangle |\phi_l\rangle$, then $\lim_{T \rightarrow \infty} \bar{P}_T(j|\alpha_0) = \frac{1}{n}$ where n is the size of the transition matrix.

To prove theorem 2, we need the following facts about the matrix D and a symmetric transition matrix P :

Lemma 1 Provide that w is an eigenvector of D with the corresponding eigenvalue $\lambda \neq \pm 1$, then it is true that $\langle A^\dagger S \alpha_0, w \rangle = \lambda \frac{\sum_l w(l)}{\sqrt{n}}$.

Proof Note that $\langle \psi_j | S \psi_l \rangle = \langle \sum_k \sqrt{p_{jk}} |jk\rangle, \sum_k \sqrt{p_{lk}} |kl\rangle \rangle = \sqrt{p_{jl} p_{lj}}$. Then we have $\langle A^\dagger S \alpha_0, w \rangle = \langle \sum_j |j\rangle \langle \phi_j | S \frac{1}{\sqrt{n}} \sum_l |\phi_l\rangle, w \rangle = \frac{1}{\sqrt{n}} \sum_j \langle \sum_l d_{jl}, w(l) \rangle = \lambda \frac{\sum_j w(j)}{\sqrt{n}}$

Lemma 2 If P is symmetric and w is an eigenvector corresponding to the eigenvalue $\lambda \neq 1$, then $\sum_i w(i) = 0$.

Proof We denote $\vec{1} = (1, 1, \dots, 1)^T$. Note that $\sum_i w(i) = \vec{1}^T P w = \lambda \vec{1}^T w = \lambda \sum_i w(i)$, this implies that $\sum_i w(i) = 0$.

Lemma 3 Provided that P is symmetric. $u_0 = \frac{1}{\sqrt{n}} \vec{1}$. If u is also an eigenvector of P with eigenvalue 1 and $\langle u, u_0 \rangle = 0$, then $\langle \alpha_0, Au \rangle = 0$.

Proof Note that $\sum_i u(i) = 0$ and $\langle \alpha_0, Au \rangle = \sum_i u(i)/\sqrt{n}$, so $\langle \alpha_0, Au \rangle = 0$.

Proof of theorem 2 To make the proof more readable, we recall some notations used before. For the given transition matrix P , the associated matrix D is defined by Eq.(1). Its spectral decomposition is assumed to be $D = \sum_r \lambda_r |w_r\rangle \langle w_r| + \sum_s |u_s\rangle \langle u_s| - \sum_t |v_t\rangle \langle v_t|$ where $\lambda_r (\neq \pm 1)$, 1 and -1 are the eigenvalues of D , $\{|w_r\rangle, |u_s\rangle, |v_t\rangle\}$ is an *orthonormal* basis for \mathcal{H}_V . Each $|w_r\rangle$ is an eigenvector of D with eigenvalue λ_r , $|u_s\rangle$ and $|v_t\rangle$ are eigenvectors of D with eigenvalues 1 and -1 , respectively.

We compute the values of $\langle \alpha_0 | \phi \rangle$ and $\langle |jk\rangle, \phi \rangle$ as follows:

1) $|\phi\rangle$ is an eigenvector of U with the corresponding eigenvalue 1. In this case, $|\phi\rangle = A|u\rangle$ where $|u\rangle$ is an eigenvector of D with the corresponding eigenvalue 1. Then $\langle\alpha_0|\phi\rangle = \langle\frac{1}{\sqrt{n}}\sum_{j=1}^n|\psi_j\rangle|A|u\rangle = \sum_i u(i)/\sqrt{n}$.

2) $|\phi\rangle$ is an eigenvector of U with the corresponding eigenvalue -1 . In this case, $|\phi\rangle = A|v\rangle$ where $|v\rangle$ is an eigenvector of D with the corresponding eigenvalue -1 . Then $\langle\alpha_0|\phi\rangle = \langle\frac{1}{\sqrt{n}}\sum_{j=1}^n|\psi_j\rangle|A|v\rangle = \sum_i v(i)/\sqrt{n}$.

3) $|\phi\rangle$ is an eigenvector of U with the corresponding eigenvalue $e^{\pm i \arccos \lambda_r} (\neq \pm 1)$. In this case, $|\phi\rangle = A|w\rangle - e^{\pm i \arccos \lambda} SA|w\rangle$ where $|w\rangle$ is an eigenvector of D with the corresponding eigenvalue λ . Then, by Lemma 1, we have $\langle\alpha_0|\phi\rangle = \langle\frac{1}{\sqrt{n}}\sum_{j=1}^n|\psi_j\rangle|A|w\rangle - e^{\pm i \arccos \lambda_r} SA|w\rangle = \frac{\sum_l w(l)(1-\lambda e^{-i \arccos(\lambda)})}{\sqrt{2(1-\lambda^2)n}}$.

4) $|\phi\rangle$ is an eigenvector of U with the corresponding eigenvalue 1. In this case, $|\phi\rangle = A|u\rangle$ where $|u\rangle$ is an eigenvector of D with the corresponding eigenvalue 1. Then $\langle|jk\rangle, \phi\rangle = \langle A^\dagger|jk\rangle, u\rangle = \sqrt{p_{jk}}u(j)$.

Applying the values of $\langle\alpha_0|\phi\rangle$ we computed above and Lemma 2, we conclude that

$$\lim_{T \rightarrow \infty} \bar{P}_T(j|\alpha_0) = \sum_k \sum_{l,m} \langle\alpha_0|\phi_l\rangle \langle j \otimes k|\phi_l\rangle \langle\phi_m|\alpha_0\rangle \langle\phi_m|j \otimes k\rangle$$

where the first sum is over all values of k , and the second sum is only on pairs l, m such that $\mu_l = \mu_m = 1$.

By Lemma 3, the aforesaid sum is further reduced to be $\bar{P}_\infty(j|\alpha_0) = \sum_k \langle\alpha_0|Au_0\rangle \langle j \otimes k|Au_0\rangle \langle Au_0|\alpha_0\rangle \langle Au_0|j \otimes k\rangle$ where the sum is over all values of k , and $u_0 = \frac{1}{\sqrt{n}}(1, 1, \dots, 1)^T$. Applying the items 1 and 4 to $\bar{P}_\infty(j|\alpha_0)$, we have that $\bar{P}_\infty(j|\alpha_0) = \frac{1}{n}$. This completes the proof.

Results presented on Theorems 1 and 2 encourage us to pursue further analytical expressions for long-term behavior of probability distributions as, in addition to mathematically characterizing quantum Markov chains on different graphs, those expressions will be useful for describing the asymptotic behavior of new quantum Markov chain-based algorithms. As an example of further developments, we envision the analysis of non-regular graphs for quantum PageRank algorithms like those numerically studied in [48, 55]).

When the transition matrix of a Markov chain is not symmetric, our preliminary study shows that the asymptotic mean probability distribution (AMPD) of MCBQW has an intimate relationship with the underlying Markov chains, for instance the AMPD is identical with the

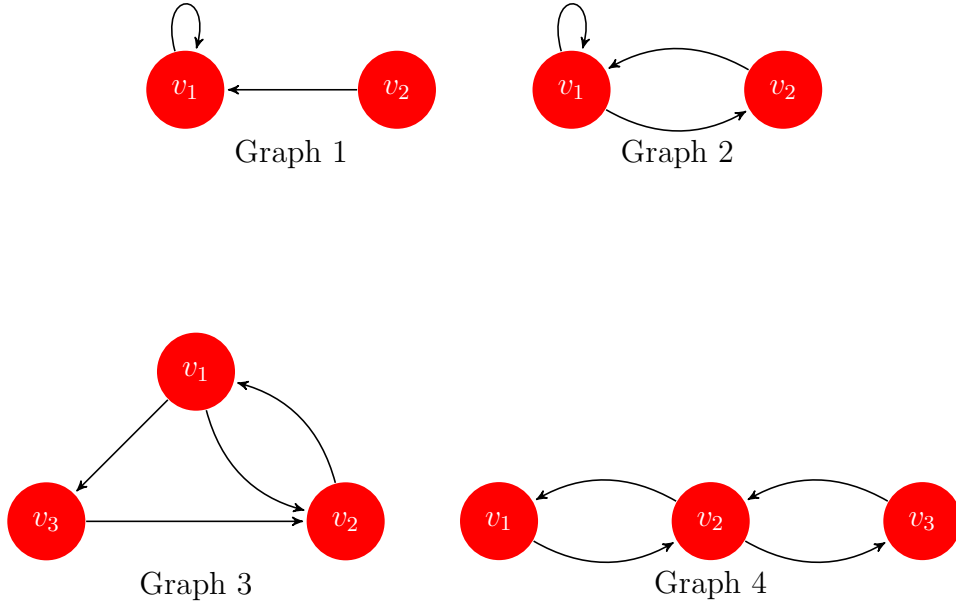


Figure 1: Four Directed Graphs

stationary distribution of the underlying Markov chain in some cases, and it is not in other cases. In what follows, we present the study on the probability distributions of some simple MCBQW.

For a directed graph G , let us adopt the usual Markov chains associated with G . The transition matrix of the Markov chain is $P = D_{in}^{-1}A$ where A is the adjacency matrix associated with the edges incident at various nodes, and where D_{in} is the degree matrix associated with edges incident at various nodes. To avoid unpleasant complications and to permit us more easily to illustrate the asymptotic mean probability distribution of MCBQW and some basic attributes of the underlying Markov chains [56], we concede, in this showcase, to confine our attention to quantum walks and Markov chains on four simple directed graphs (see Figure 1). A summary of the study are shown in the table below.

Table I Probability Distributions: MCBQW vs MC

	Graph 1	Graph 2	Graph 3	Graph 4
P (MC)	$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} .5 & .5 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & .5 & .5 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 & 0 \\ .5 & 0 & .5 \\ 0 & 1 & 0 \end{bmatrix}$
Properties of MC.	redu, reve	ergodic, reve	ergodic, not reve	irred, periodic, reve
π (MC)	$(1, 0)$	$(\frac{2}{3}, \frac{1}{3})$	$(\frac{2}{5}, \frac{2}{5}, \frac{1}{5})$	$(\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$
\bar{P}_∞ (QW)	$(\frac{3}{4}, \frac{1}{4})$	$(\frac{2}{3}, \frac{1}{3})$	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	$(\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$

Notes: In this table, P is the transition matrix of the Markov chain associated with a graph, π is the stationary probability distribution of a Markov chain, \bar{P}_∞ is the asymptotic mean probability distribution of MCBQW, “redu” stands for “reducible”, “irred” stands for “irreducible”, and “reve” stands for “reversible”.

4 Weak limits for MCBQW on the line

MCBQW can be extended to infinite lattices. As far as we are aware, there is only one publication in the literature concerning MCBQW on an infinite lattice [50], where the relationship between the asymptotic mean probability distribution of MCBQW and the recurrence of the underlying random walk on the half line is discussed. No publication has ever treated weak limits, the fundamental statistical property for MCBQW on an infinite lattice. In this work we confine our attention to one-dimensional lattice (a line). The underlying Markov chain is a lazy random walk (see Figure 2).

Let P denote the governing probability operator for the random walk. The transition rules of P are as follows:

$$P|x\rangle = \frac{1}{3}|x-1\rangle + \frac{1}{3}|x\rangle + \frac{1}{3}|x+1\rangle \text{ for } x \in \mathbb{Z}. \quad (3)$$

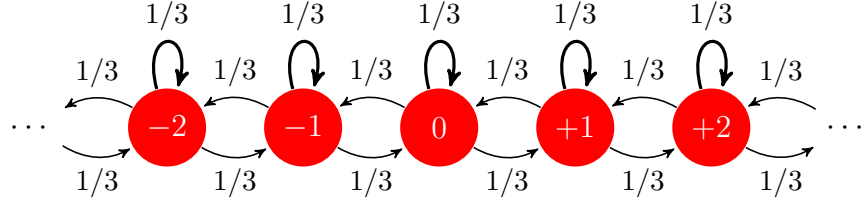


Figure 2: A lazy random walk on the line

In this scenario, the vector states, the orthogonal projector and the swap operator are given as follows: $|\psi_j\rangle = \frac{\sqrt{3}}{3}|j\rangle \otimes |j-1\rangle + \frac{\sqrt{3}}{3}|j\rangle \otimes |j\rangle + \frac{\sqrt{3}}{3}|j\rangle \otimes |j+1\rangle$ for $j \in \mathbb{Z}$, $\Pi = \sum_{j=-\infty}^{\infty} |\psi_j\rangle\langle\psi_j|$, $S = \sum_{j,k} |j \otimes k\rangle\langle k \otimes j|$.

The unitary operator $U = S(2\Pi - 1)$ for MCBQW on the line is encoded in the following formula:

$$U|x, x-1\rangle = -\frac{1}{3}|x-1, x\rangle + \frac{2}{3}|x, x\rangle + \frac{2}{3}|x+1, x\rangle, U|x, x\rangle = \frac{2}{3}|x-1, x\rangle - \frac{1}{3}|x, x\rangle + \frac{2}{3}|x+1, x\rangle, \\ U|x, x+1\rangle = \frac{2}{3}|x-1, x\rangle + \frac{2}{3}|x, x\rangle - \frac{1}{3}|x+1, x\rangle.$$

The “overall” state space of the system is $\mathcal{H} = \text{span}\{|j\rangle \otimes |k\rangle, j, k \in \mathbb{Z}\}$ in terms of which a general state of the system may be expressed by the formula:

$$\psi = \sum_{j \in \mathbb{Z}} \sum_{k \in \mathbb{Z}} \psi(j, k) |j\rangle \otimes |k\rangle.$$

Given $\psi_0 \in \mathcal{H}$, where $||\psi_0|| = 1$, the expression $\psi_t = U^t \psi_0$ is the state of the MCBQW at time t . Let $\psi_t = \sum_{j \in \mathbb{Z}} (\psi_t(j, j-1)|j\rangle \otimes |j-1\rangle + \psi_t(j, j)|j\rangle \otimes |j\rangle + \psi_t(j, j+1)|j\rangle \otimes |j+1\rangle)$ be the wave function for the MCBQW at time t . Then the probability $p_t(j)$ of finding the walker at the position j at time t is given by the standard formula

$$p_t(j) = |\psi_t(j, j-1)|^2 + |\psi_t(j, j)|^2 + |\psi_t(j, j+1)|^2,$$

where $|\cdot|$ indicates the modulus of a complex number.

Let $\Psi_t(x) \equiv [\psi_t(x, x-1), \psi_t(x, x), \psi_t(x, x+1)]^T$ represent the amplitude of the wave function of the MCBQW at position j and time t .

The spatial Fourier transform of $\Psi_t(x)$ is defined by

$$\widehat{\Psi}_t(k) = \sum_{j \in \mathbb{Z}} \Psi_t(x) e^{ikx}.$$

Thus, given the initial state $\widehat{\Psi}_0(k)$, the Fourier dual of the wave function of the MCBQW system is expressed by

$$\widehat{\Psi}_t(k) = U(k)^t \widehat{\Psi}_0(k), \quad (4)$$

where the total evolution operator $U(k)$ is given by

$$U(k) = \begin{bmatrix} 0 & 0 & e^{ik} \\ 0 & 1 & 0 \\ e^{-ik} & 0 & 0 \end{bmatrix} \begin{bmatrix} -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \end{bmatrix} \quad (5)$$

This formulation for the unitary operator U lends us a tool to tackle the weak limit of the QW. In what follows, we shall investigate weak limits and limiting distributions of MCBQW on infinite lattices.

The three eigenvalues of $U(k)$ are $\lambda_1 = -1$, $\lambda_2 = \frac{1}{3} + \frac{2}{3} \cos k + \frac{2}{3} i \sqrt{2 - \cos^2 k - \cos k}$, and $\lambda_3 = \frac{1}{3} + \frac{2}{3} \cos k - \frac{2}{3} i \sqrt{2 - \cos^2 k - \cos k}$. Therefore we have

$$\overline{\lambda_1} D \lambda_1 = 0, \quad \overline{\lambda_2} D \lambda_2 = -\overline{\lambda_3} D \lambda_3 = \frac{\sin k}{\sqrt{2 - \cos^2 k - \cos k}} \quad (6)$$

Here, $D = -id/dk$ denote the position operator in k -space. The corresponding unit eigenvectors are given below:

$$v_1 = \frac{1}{\sqrt{4 + 2 \cos k}} \begin{bmatrix} e^{ik} \\ -1 - e^{ik} \\ 1 \end{bmatrix}, \quad v_2 = \frac{1}{\sqrt{c_2}} \begin{bmatrix} e^{ik} \left[-3 - 2 \cos k - \frac{2\sqrt{2 - \cos^2 k - \cos k} \sin k}{1 - \cos k} \right] \\ (-\sin k - \sqrt{2 - \cos^2 k - \cos k}) \left(\frac{\sin k}{1 - \cos k} + i \right) \\ 1 \end{bmatrix}, \quad (7)$$

$$v_3 = \frac{1}{\sqrt{c_3}} \begin{bmatrix} e^{ik} \left[-3 - 2 \cos k + \frac{2\sqrt{2 - \cos^2 k - \cos k} \sin k}{1 - \cos k} \right] \\ (-\sin k + \sqrt{2 - \cos^2 k - \cos k}) \left(\frac{\sin k}{1 - \cos k} + i \right) \\ 1 \end{bmatrix}. \quad (8)$$

Here, $c_2 = 12 + 4 \cos 2k + 12 \cos k - 8 \sin k \sqrt{2 - \cos^2 k - \cos k} + \frac{16 \sin^2 k + 24 \sin k \sqrt{2 - \cos^2 k - \cos k}}{1 - \cos k}$, and $c_3 = 12 + 4 \cos 2k + 12 \cos k + 8 \sin k \sqrt{2 - \cos^2 k - \cos k} + \frac{16 \sin^2 k - 24 \sin k \sqrt{2 - \cos^2 k - \cos k}}{1 - \cos k}$.

According to the methods by Grimmett *et al.* [57], the moments of the position distribution are given as

$$E(X_t^r) = \int_0^{2\pi} \langle \widehat{\Psi}_t(k), D^r \widehat{\Psi}_t(k) \rangle \frac{dk}{2\pi}. \quad (9)$$

Using the standard calculations, we arrive at, as $t \rightarrow \infty$,

$$E[(X_t/t)^r] = \int_0^{2\pi} \sum_{j=1}^3 \left(\frac{D\lambda_j(k)}{\lambda_j(k)} \right)^r |\langle v_j(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} + O(t^{-1}). \quad (10)$$

By the method of moments (see [57] and references therein), we can derive the following limit theorem.

Theorem 3. Suppose the MCBQW, induced by the lazy random walk on the line, is launched from the origin in the initial state $\Psi_0 = \alpha|0, -1\rangle + \beta|0, 0\rangle + \gamma|0, 1\rangle$, where $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. For $y \in [-1, 1]$, let $\delta_0(y)$ denote the *point mass at the origin* and let $I_{(a,b)}(y)$ denote the *indicator function* of the real interval (a, b) . Then, as $t \rightarrow \infty$, the normalized position distribution $f_t(y)$ associated with $\frac{1}{t}X_t$ converges, in the sense of a weak limit, to the density function

$$f(y) = c\delta_0(y) + \frac{I_{(-\frac{\sqrt{6}}{3}, \frac{\sqrt{6}}{3})}(y)}{2\pi(1-y^2)\sqrt{2-3y^2}} \left(\sum_{j=0}^2 a_j y^j \right). \quad (11)$$

In the above formula, the coefficients c , a_0 , a_1 and a_2 are given by

$$\begin{cases} c = \frac{\sqrt{3}}{6} + \frac{\sqrt{3}-3}{3}\text{Re}(\alpha\bar{\beta}) + \frac{3-2\sqrt{3}}{3}\text{Re}(\alpha\bar{\gamma}) + \frac{\sqrt{3}-3}{3}\text{Re}(\beta\bar{\gamma}) + \frac{2-\sqrt{3}}{2}|\beta|^2 \\ a_0 = 1 + |\beta|^2 + 2\text{Re}(\alpha\bar{\gamma}) \\ a_1 = 2|\alpha|^2 - 2|\gamma|^2 + 2\text{Re}(\alpha\bar{\beta}) - 2\text{Re}(\beta\bar{\gamma}) \\ a_2 = 1 - 3|\beta|^2 + 2\text{Re}(\alpha\bar{\beta}) - 4\text{Re}(\alpha\bar{\gamma}) + 2\text{Re}(\beta\bar{\gamma}) \end{cases}$$

Where $\text{Re}(z)$ is the real part of a complex number z .

It is noteworthy that a similar type of quantum walk on the line driven by the Grover coin has been studied, and its weak limit was obtained [58, 59]. We would like to point out that MCBQW appears to spread faster than the coin-driven quantum walk although the weak limits of these two types of quantum walks are similar. The aforesaid claim is based on the following simple observation: The indicator function in a formula of density function shows the interval over which the quantum walks prevails. The indicator function of MCBQW discussed in this paper has a wider interval than its counterpart-the quantum walks on the line driven by the Grover coin.

Another attention we would like to draw to MBQW is that this type of quantum walks may have a phenomenon called *localization* due to the degeneration of eigenvalues of the time evolution operator ($\lambda_1 = -1$) [60]. We stress that the degeneration of eigenvalues is only

the necessary condition for *localization*, which in fact also depends upon the initial state of MCBQW. For instance, we consider the case when $\alpha = \beta = \gamma = \frac{\sqrt{3}}{3}$. A direct calculation shows that the density function in Theorem 3 becomes

$$f(y) = \frac{I_{(-\frac{\sqrt{6}}{3}, \frac{\sqrt{6}}{3})}(y)}{\pi(1-y^2)\sqrt{2-3y^2}}. \quad (12)$$

This is the case where *localization* does not occur as the coefficient $c = 0$ in Eq. (11).

Proof of theorem 3. We begin with the moments of the position distribution:

$$E[(X_t/t)^r] = \int_0^{2\pi} \sum_j \left(\frac{D\lambda_j(k)}{\lambda_j(k)} \right)^r |\langle v_j(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} + O(t^{-1}). \quad (13)$$

By the method of moments (see [57] and references therein), the weak limit of X_t/t exists. Let Y be this weak limit. Then we have

$$P(Y \leq y) = \int_{h^{-1}(k,j)((-\infty,y])} \sum_{j=1}^3 |\langle v_j(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \quad (14)$$

where $h(k, j) = \overline{\lambda_j} D\lambda_j(k)$ given by Eq. (6).

According to Eq. (6), the probability distribution function in Eq. (14) can be written as

$$\begin{aligned} P(Y \leq y) &= H(y) \int_0^{2\pi} |\langle v_1(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \\ &+ \int_{\arccos \frac{2y^2-1}{1-y^2}}^{2\pi} |\langle v_2(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \\ &+ \int_0^{2\pi - \arccos \frac{2y^2-1}{1-y^2}} |\langle v_3(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi}, \text{ for } y \geq 0. \end{aligned} \quad (15)$$

$$\begin{aligned} P(Y \leq y) &= H(y) \int_0^{2\pi} |\langle v_1(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \\ &+ \int_{2\pi - \arccos \frac{2y^2-1}{1-y^2}}^{2\pi} |\langle v_2(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \\ &+ \int_0^{\arccos \frac{2y^2-1}{1-y^2}} |\langle v_3(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi}, \text{ for } y < 0. \end{aligned} \quad (16)$$

Here $H(y)$ is *Heaviside function*, which is the cumulative distribution function of $\delta_0(y)$.

After taking derivatives of both sides of Eqs. (15) and (16) with respect to y , we obtain the density (in both cases when $y \geq 0$ and $y < 0$) as follows

$$\begin{aligned}
f(y) &= \frac{dP(Y \leq y)}{dy} \\
&= \delta_0(y) \int_0^{2\pi} |\langle v_1(k), \widehat{\Psi}_0(k) \rangle|^2 \frac{dk}{2\pi} \\
&\quad + \frac{1}{\pi(1-y^2)\sqrt{2-3y^2}} |\langle v_2(k), \widehat{\Psi}_0(k) \rangle|_{k=\arccos \frac{2y^2-1}{1-y^2}}^2 \\
&\quad + \frac{1}{\pi(1-y^2)\sqrt{2-3y^2}} |\langle v_3(k), \widehat{\Psi}_0(k) \rangle|_{k=2\pi-\arccos \frac{2y^2-1}{1-y^2}}^2
\end{aligned} \tag{17}$$

Applying Eqs. (7) and (8) to simplify Eq. (17), one can obtain the density function $f(y)$ given in Eq. (11)

5 Outlook

The application of MCBQW to transport for large classes of physical phenomena involving different types of networks has turned out to be successful in recent years such as [48, 55]. Except for Theorems 1 and 2 shown in this article, however, only little is known about the detailed relations between properties of underlying Markov chains and the asymptotic average probability distribution of MCBQW. Therefore, a thorough investigation of the influence of different properties of Markov chains aspects on the dynamics is clearly necessary.

Based on the preliminary studies shown above, one may proceed to investigate the things outlined below:

1. If the Markov chain is irreducible (the directed graph is strongly connected) and reversible, is the mean probability distribution of MCBQW identical to the stationary probability of MC. Actually, *irreducibility* guarantees the existence and uniqueness of the stationary distribution of MC. The condition can be relaxed, we then may restate this conjecture in the following manner: *If the Markov chain has a unique stationary probability distribution and is reversible, then the mean probability distribution of MCBQW is identical to the stationary distribution of MC.*

2. If the Markov chain is irreducible and is not reversible, then is the mean probability distribution of MCBQW uniform?

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